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INTERSTELLAR ISOTHIOCYANIC ACID

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ABSTRACT

Isothiocyanic acid (HNCS) has been identified in Sgr B2 from millimeter-wave spectral line observations. We have definitely detected three rotational lines, and have probably detected two others. The rotational temperature of HNCS in Sgr B2 is 14 ± 5 K, its column density is 2.5 ± 1.0×10^{13} cm^{-2}, and its abundance relative to HNCO is consistent with the cosmic S/O ratio, 1/42.
Subject headings: interstellar: molecules

The detection of methyl mercaptan (CH_3SH) in Sgr B2 (Linke *et al.* 1979) encouraged us to search for sulfur analogs of other interstellar oxygen-containing molecules. Isothiocyanic acid (HNCS) was an obvious candidate. Its millimeter-wave spectrum can be accurately calculated from existing laboratory data (Kewley *et al.* 1963), and its oxygen analog, isocyanic acid (HNCO), is conspicuous in Sgr B2. With the Bell Laboratories 7 m telescope the intensities of the stronger millimeter-wave lines of HNCO are about 3 K; if the HNCS/HNCO ratio equals the cosmic ratio, 1/42, HNCS lines would be expected to be about 0.05 K. Lines as weak as this are readily detected with the cryogenic receivers now on the 7 m telescope.

The identification of HNCS, however, was more difficult than expected because receiver noise was not the only source of uncertainty. At a flux level of a few hundredths of a degree Kelvin, the spectrum of Sgr B2 is sufficiently rich in unidentified lines for misidentifications to occur. The first line of HNCS we observed with the 7 m telescope, $9_{09} \rightarrow 8_{08}$ at 105,558 MHz, was found to be flanked by two weak lines of unknown origin (Fig. 1), and it was only after we succeeded in observing two other rotational transitions well removed in frequency, $8_{08} \rightarrow 7_{07}$ at 93,830 MHz and $11_{0,11} \rightarrow 10_{0,10}$ at 129,013 MHz, that we were confident we had detected HNCS. Subsequently, we obtained marginal evidence for two additional lines: $12_{0,12} \rightarrow 11_{0,11}$ at 140,740 MHz (also observed with the 7 m telescope), and $7_{07} \rightarrow 6_{06}$ at 82,101 MHz (observed with the NRAO 36 foot (11 m) telescope). Figures 1 and 2 and Table 1 summarize the observational data. A summary of negative results in other sources is contained in Table 2.

Since long integration times were required to detect HNCS in Sgr B2, we have not mapped its distribution and so do not know its angular extent. HNCO, however, extends over at least $5' \times 5'$ in Sgr B2 (Buhl *et al.* 1973; Churchwell 1979); it is therefore likely that HNCS at least fills our $\sim 2'$ antenna beam. Analysis of our present data is based on this assumption, but the final results would not differ greatly if the HNCS source is pointlike.

Except for the hydrogen atom, HNCS is a linear molecule, and its rotational spectrum is that of a highly prolate, nearly symmetric top. Rotational levels having angular momentum about the quasi-symmetry axis ($K > 0$) lie well above the ground state ($E/k > 70$ K), and are connected to the $K = 0$ ladder by fast radiative ($\Delta K = 1$) transitions owing to the component of the molecular dipole moment perpendicular to the heavy-atom backbone. These higher levels are not appreciably populated in Sgr B2, and hence the spectrum reduces to that of the $K = 0$ ladder, which is the spectrum of a linear molecule with rotation constant $B_{\rm eff} = (B + C)/2$. The rotational partition function is given to adequate accuracy by the simple classical expression for a linear molecule, $Z = kT_{\rm rot}/hB_{\rm eff}$.

Fig. 2 is a log intensity versus rotational energy plot of the data in Table 1, similar to the one for CH_3SH presented in the preceding *Letter*. The rotational levels of HNCS, like those of CH_3SH, appear to be in approximate thermal equilibrium in Sgr B2. A least-squares fit to the expression for optically thin thermal emission lines (cf. Linke, Frerking, and Thaddeus 1979) yields for the rotational temperatures of HNCS

$$T_{\rm rot} = 14 \pm 5 \text{ K}, \tag{1}$$

and for its column density

$$N = 2.5 \pm 1.0 \times 10^{13} \text{ cm}^{-2}, \tag{2}$$

where the uncertainties are 1 σ.

The rotational temperature of HNCS agrees fairly well with that for CH_3SH, 9 ± 3 K. As already noted for CH_3SH, this is low with respect to some other molecular temperatures in Sgr B2. It is therefore possible that the rotational excitation of HNCS is subthermal, and that rotational equilibrium is only approximate.

It is interesting to compare the column density of HNCS with that of HNCO. By observing the $4_{04} \rightarrow 3_{03}$ transition of HNCO at 87,925 MHz with the 7 m telescope we have obtained essentially a *lower* limit on N(HNCO) (saturation cannot be excluded). Similarly, by setting a limit on the same transition of $H^{15}NCO$ at 85,292 MHz, and assuming that the ratio of this rare isotopic species to HNCO is the same as the terrestrial $^{15}N/^{14}N$ ratio, we have set an *upper* limit on N(HNCO) (the carbon-13 species cannot be used for this purpose since its lines lie on top of those of HNCO). These limits are

$$1.0 \times 10^{15} \lesssim N(\mathrm{HNCO}) \lesssim 5 \times 10^{15}\ \mathrm{cm}^{-2}. \quad (3)$$

Equations (2) and (3) then yield

$$1/300 \lesssim \mathrm{HNCS/HNCO} \lesssim 1/30, \quad (4)$$

a range which includes the cosmic S/O ratio, 1/42.

Isothiocyanic acid hence reinforces the general impression gained from our detection of methyl mercaptan

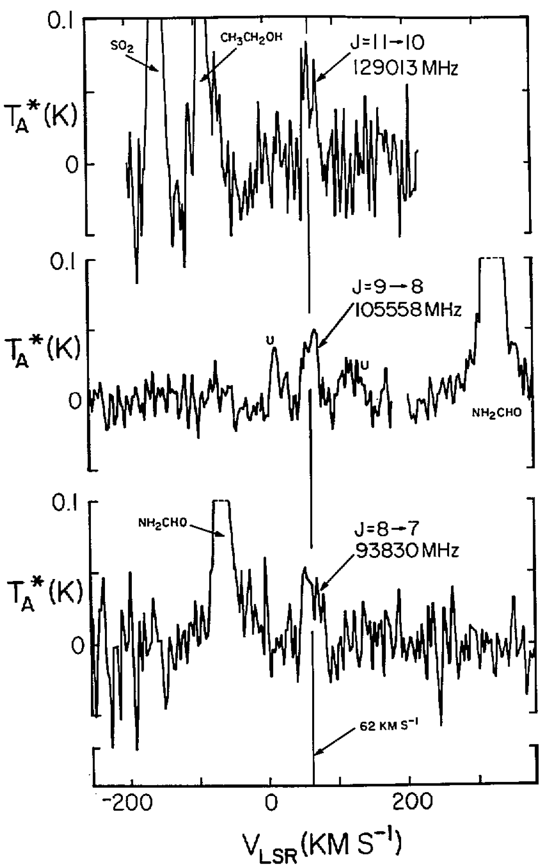

FIG. 1.—The three best-detected rotational transitions of HNCS in Sgr B2, observed with the Bell 7 m telescope at a spectral resolution of 1 MHz.

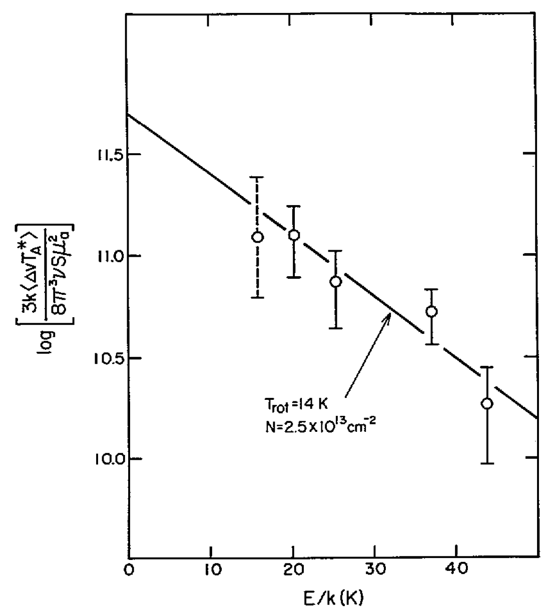

FIG. 2.—Log intensity versus rotational energy plot of HNCS data for Sgr B2. Owing to poor quality of low E/k point, the linear theoretical expression for optically thin thermal emission has been fitted only to the higher four points.

TABLE 1

ISOTHIOCYANIC ACID IN SAGITTARIUS B2[a]

Transition	ν_0 (MHz)	T_A^* (K)	v_{LSR} (km s^{-1})	Δv (km s^{-1})
$7_{07} \rightarrow 6_{06}$........	82,101.67	0.05±50%	~60	~25
$8_{08} \rightarrow 7_{07}$........	93,829.92	0.05±0.01	60±4	30±10
$9_{09} \rightarrow 8_{08}$........	105,557.95	0.05±0.01	65±3	27±9
$11_{0,11} \rightarrow 10_{0,10}$...	129,013.21	0.06±0.01	64±3	21±6
$12_{0,12} \rightarrow 11_{0,11}$...	140,740.39	0.05±0.02	~70	11±5

NOTE.—T_A^*, v_{LSR}, and Δv (full velocity width at half-intensity) have been determined when feasible by a least-squares fit of Gaussian line profiles to the observational data in Fig. 1. Uncertainties are 1 σ. Rest frequencies ν_0 are calculated from microwave constants of Kewley *et al.* 1963.

[a] $\alpha(1950) = 17^h44^m11^s$, $\delta(1950) = -28°22'30''$.

TABLE 2

HNCS NEGATIVE RESULTS

Source	Frequency (MHz)	Telescope	Spectrosc. Resolution (MHz)	Upper Limit on T_A^*(K)[a]
Ori A(KL)........	82101	11 m	1	0.10
Ori A(KL)........	105557	7 m	0.25	0.16
IRC +10216.....	82101	11 m	1	0.05
IRC +10216.....	93829	7 m	1	0.05
IRC +10216.....	105557	7 m	1	0.04
DR 21(OH)......	82101	11 m	0.25	0.20
W3(OH).........	82101	11 m	0.25	0.20

[a] Peak-to-peak receiver noise.

that the interstellar chemistry of sulfur resembles fairly closely that of oxygen—or at any rate that differences between the two chemistries are not easy to demonstrate. It will be interesting to see whether this qualified conclusion holds for other sources and other molecules. The most conspicuous remaining gap in the table of interstellar sulfur molecules is HCS^+, an ion not yet detected in the laboratory, but which we have hopes of finding on the basis of a recent *ab initio* structural calculation (Wilson 1978).

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